Measuring Conditional Dependence with Kernels

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Outline

1. Introduction

2. Characterization of conditional independence with kernels

3. Conditional dependence measure with normalized operators and its kernel-free expression.

4. Experiments

5. Concluding remarks
Introduction

“Kernel methods” for nonlinear relations

- Positive definite kernels have been used for capturing nonlinearity of original data. e.g. Support vector machine.
- Kernelization: mapping data into a functional space (RKHS) and apply linear methods on RKHS.
- Consider linear statistics (mean, variance, …) on RKHS, and their meaning on the original space.
Representing probabilities
  – Determining probabilities  (Arthur Gretton’s talk)
  – Characterizing independence  (Arthur Gretton’s talk)
  – Characterizing conditional independence

Motivation
  – Dependence among many variables
  – Conditional independence is essential for many probabilistic modeling
    e.g. graphical modeling
Positive Definite Kernel and RKHS

■ Positive definite kernel (p.d. kernel)

Ω: set. \( k : \Omega \times \Omega \to \mathbb{R} \)

\( k \) is positive definite if \( k(x, y) = k(y, x) \) and for any \( n \in \mathbb{N}, \ x_1, \ldots x_n \in \Omega \)
the matrix \( \left( k(x_i, x_j) \right)_{i,j} \) (Gram matrix) is positive semidefinite.

- Example: Gaussian RBF kernel
  \[ k(x, y) = \exp\left(-\frac{\|x - y\|^2}{\sigma^2}\right) \]

■ Reproducing kernel Hilbert space (RKHS)

\( k \): p.d. kernel on \( \Omega \).

\( \iff \exists \ H \colon \text{reproducing kernel Hilbert space (RKHS)} \)

1) \( k(\cdot, x) \in H \) for all \( x \in \Omega \).

2) \( \operatorname{Span}\{k(\cdot, x) | x \in \Omega\} \) is dense in \( H \).

3) \( \langle k(\cdot, x), f \rangle_H = f(x) \) (reproducing property)
### Functional data (feature map)

\[ \Phi : \Omega \to H, \quad x \mapsto k(\cdot, x) \quad \text{i.e.} \quad \Phi(x) = k(\cdot, x) \]

\[ \langle \Phi(x), f \rangle = f(x) \quad \text{(reproducing property)} \]

Data: \( X_1, \ldots, X_N \) \( \to \) \( \Phi(X_1), \ldots, \Phi(X_N) \) : functional data

### Why RKHS?

- By the reproducing property, computation of the inner product on RKHS does not need expansion by basis functions.

\[ f(\cdot) = \sum_i a_i k(\cdot, x_i), \quad g(\cdot) = \sum_j b_j k(\cdot, x_j) \]

\[ \Rightarrow \quad \langle f, g \rangle = \sum_{i,j} a_i b_j k(x_i, x_j) \]

Advantageous for high-dimensional data of small sample size.
Representing Nonlinear Dependence

Kernel Statistics: linear statistics on RKHS

$X, Y$: general random variables on $\Omega_X$ and $\Omega_Y$, resp.

Prepare RKHS $(H_X, k_X)$ and $(H_X, k_X)$ defined on $\Omega_X$ and $\Omega_Y$, resp.

Define random variables on the RKHS $H_X$ and $H_Y$ by

$\Phi_X(X) = k_X(\cdot, X)$  \quad $\Phi_Y(Y) = k_Y(\cdot, Y)$

- Covariance

$\Sigma_{XY} \equiv E[(\Phi_Y(Y) - \mu_X)(\Phi_X(X) - \mu_Y)^T]$  \quad $\Sigma_{XY} = O \iff X \perp Y$

- Conditional covariance

$\Sigma_{YX|Z} \equiv \Sigma_{XY} - \Sigma_{YZ} \Sigma_{ZZ}^{-1} \Sigma_{ZX}$  \quad $\Sigma_{YX|Z} = O \iff X \perp Y \mid Z$

- c.f. Gaussian variables

$V_{XY} = O \iff X \perp Y$

$V_{YX|Z} = O \iff X \perp Y \mid Z$
Richness Assumption on RKHS

\( k \): kernel on a measurable space \((\Omega, \mathcal{B})\). \( H \): associated RKHS.

**Assumption (A):**
\[ \exists q \geq 1. \quad H + \mathbb{R} \text{ is dense in } L^q(P) \text{ for any probability } P \text{ on } (\Omega, \mathcal{B}), \]

- RKHS can approximates various functions such as the index function of a measurable set, polynomials, and \( e^{-\frac{1}{2} \omega^T x} \).

- Example: Gaussian kernel on the entire \( \mathbb{R}^m \)
  \[ k_G(x, y) = \exp \left( -\frac{\|x - y\|^2}{2\sigma^2} \right) \]

  Laplacian kernel on the entire \( \mathbb{R}^m \)
  \[ k_L(x, y) = \exp \left( -\lambda \sum_{i=1}^{m} |x_i - y_i| \right) \]
Covariance on RKHS

- **Definition**: cross-covariance operator
  
  $X, Y$ : general random variables on $\Omega_X$ and $\Omega_Y$, resp.

  Prepare RKHS $(H_X, k_X)$ and $(H_X, k_X)$ defined on $\Omega_X$ and $\Omega_Y$, resp.

  There is a unique operator $\Sigma_{XY} : H_X \to H_Y$ such that

  $$\langle g, \Sigma_{XY} f \rangle = E[g(Y)f(X)] - E[g(Y)]E[f(X)] \quad (= \text{Cov}[f(X), g(Y)])$$

  for all $f \in H_X, g \in H_Y$

- **Independence by cross-covariance operator**

  Under (A),

  $X$ and $Y$ are independent $\iff \Sigma_{XY} = O$

  $$E[g(Y)f(X)] = E[g(Y)]E[f(X)]$$

  - *c.f. Characteristic function*

    $X \perp Y \iff E_{XY}[e^{\sqrt{-1}(uX+vY)}] = E_X[e^{\sqrt{-1}uX}]E_Y[e^{\sqrt{-1}vY}]$
Conditional Covariance on RKHS

- **Conditional Cross-covariance operator**

  $X, Y, Z : \text{random variables on } \Omega_X, \Omega_Y, \Omega_Z \text{ (resp.)}$

  $(H_X, k_X), (H_Y, k_Y), (H_Z, k_Z) : \text{RKHS defined on } \Omega_X, \Omega_Y, \Omega_Z \text{ (resp.)}$

  - Conditional cross-covariance operator $H_X \rightarrow H_Y$
    
    $\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX}$

  - Conditional covariance operator
    
    $\Sigma_{YY|Z} \equiv \Sigma_{YY} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZY}$

  - Note: $\Sigma_{ZZ}^{-1}$ may not exist. But, we have the decomposition
    
    $\Sigma_{YX} = \Sigma_{YY}^{1/2}W_{YX}\Sigma_{XX}^{1/2}$  \quad \text{with operator norm } \|W_{YX}\| \leq 1$

  Rigorously, define $\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YY}^{1/2}W_{YZ}W_{ZX}\Sigma_{XX}^{1/2}$
Relation with regression error

Theorem (FBJ’06)

\( Y, Z \) : random variables on \( \Omega_Y, \Omega_Z \) (resp.).

\( (H_Y, k_Y), (H_Z, k_Z) \) : RKHS defined on \( \Omega_Y, \Omega_Z \) (resp.).

\[
\left\langle g, \Sigma_{YY|Z} f \right\rangle = \inf_{f \in H_Z} E \left| (g(Y) - E[g(Y)]) - (f(Z) - E[f(Z)]) \right|^2 \\
= \inf_{f \in H_Z} \text{Var} \left[ g(Y) - f(Z) \right] \quad (\forall g \in H_Y)
\]

c.f. for Gaussian variables,

\[
b^T V_{YY|Z} b = \min_a \left| b^T \tilde{Y} - a^T \tilde{Z} \right|^2 \quad (\tilde{Y} = Y - E[Y], \tilde{Z} = Z - E[Z])
\]

Residual error of linear regression is given by the conditional covariance matrix.
– Rough sketch of the proof

\[
E\left[(g(Y) - E[g(Y)]) - (f(Z) - E[f(Z)])\right]^2
\]

\[
= \langle f, \Sigma_{ZZ} f \rangle - 2 \langle f, \Sigma_{ZY} g \rangle + \langle g, \Sigma_{YY} g \rangle
\]

\[
= \left\| \Sigma_{ZZ}^{1/2} f \right\|^2 - 2 \langle f, \Sigma_{ZZ}^{1/2} W_{ZY} \Sigma_{YY}^{1/2} g \rangle + \left\| \Sigma_{YY}^{1/2} g \right\|^2
\]

\[
= \left\| \Sigma_{ZZ}^{1/2} f - W_{ZY} \Sigma_{YY}^{1/2} g \right\|^2 + \left\| \Sigma_{YY}^{1/2} g \right\|^2 - \left\| W_{ZY} \Sigma_{YY}^{1/2} g \right\|^2
\]

\[
= \left\| \Sigma_{ZZ}^{1/2} f - W_{ZY} \Sigma_{YY}^{1/2} g \right\|^2 + \langle g, \left( \Sigma_{YY} - \Sigma_{YY}^{1/2} W_{YZ} W_{ZY} \Sigma_{YY}^{1/2} \right) g \rangle
\]

This part can be arbitrary small by choosing \( f \).
Relation with conditional covariance

**Theorem** (FBJ’06, Sun et al. ’07)

Let $X, Y, Z$ be random variables on $\Omega_X, \Omega_Y, \Omega_Z$ (resp.).

$(H_X, k_X), (H_Y, k_Y), (H_Z, k_Z)$: RKHS defined on $\Omega_X, \Omega_Y, \Omega_Z$ (resp.).

Assume

$$H_Z + \mathbb{R} : \text{dense in } L^2(P_Z)$$

then,

$$\langle g, \Sigma_{Y|Z} f \rangle = E[\text{Cov}[g(Y), f(X) | Z]] \quad (\forall f \in H_X, g \in H_Y)$$

- *c.f.* for Gaussian variable

$$a^T V_{XY|Z} b = \text{Cov}[a^T X, b^T Y | Z]$$

(not dependent on the value of $z$)
– Sketch of the proof for the simpler case of $X = Y$ and $f = g$,
i.e. $\langle g, \Sigma_{YY|Z} g \rangle = E[Var[g(Y) \mid Z]]$

\begin{enumerate}
\item \textbf{Lemma}
\end{enumerate}

\begin{equation}
Var[Y] = Var_X [E_Y [Y \mid X]] + E_X [Var_{Y|X} [Y \mid X]]
\end{equation}

\begin{align*}
\langle g, \Sigma_{YY|Z} g \rangle &= \inf_{f \in H_Z} Var[g(Y) - f(Z)] \\
&= \inf_{f \in H_Z} \{Var[E[g(Y) - f(Z) \mid Z]] + E[Var[g(Y) - f(Z) \mid Z]]\} \\
&= \inf_{f \in H_Z} Var[E[g(Y) \mid Z] - f(Z)] + E[Var[g(Y) \mid Z]] \\
&\in L^2(P_Z) \\
&= 0 + E[Var[g(Y) \mid Z]] \quad \text{(by denseness assumption)}
\end{align*}
Conditional Independence

Theorem (FBJ04, Sun et al 07)

Under (A),

$$\Sigma_{YX|Z} = O \iff P_{YX} = E_Z[P_{Y|Z} \otimes P_{X|Z}]$$

where $E_Z[P_{Y|Z} \otimes P_{X|Z}]$ is a probability on $\Omega_X \times \Omega_Y$ defined by

$$E_Z[P_{Y|Z} \otimes P_{X|Z}](B \times A) = \int P_{Y|Z}(B \mid Z = z)P_{X|Z}(A \mid Z = z)dP_Z(z)$$

With p.d.f.

$$E_Z[P_{Y|Z} \otimes P_{X|Z}](A \times B) = \int \int_A p_{X|Z}(x \mid z)d\mu_1(x)\int_B p_{Y|Z}(y \mid z)d\mu_2(y)dP_Z(z)$$

Remark: The assertion $P_{YX} = E_Z[P_{Y|Z} \otimes P_{X|Z}]$ is weaker than the conditional independence $P_{YX|Z} = P_{Y|Z} \otimes P_{X|Z}$

C.f. for Gaussian variables

$$\Sigma_{YX|Z} = O \iff X \perp \!\!\!\!\perp Y \mid Z$$
- Proof of \( \Sigma_{Y|Z} = O \Rightarrow P_{YX} = E_Z[P_{Y|Z} \otimes P_{X|Z}] \)

\( \Sigma_{Y|Z} = O \) means \( E[\text{Cov}[g(Y), f(X) | Z]] = 0 \)

\( \Rightarrow \ E[E[g(Y)f(X) | Z]] = E[E[g(Y) | Z]E[f(X) | Z]] \)

\( \Rightarrow \ E_{P_{XY}}[g(Y)f(X)] = E_{E_Z[P_{Y|Z} \otimes P_{X|Z}]}[g(Y)f(X)] \quad \forall f \in H_X, g \in H_Y \)

Under (A), by approximating the index function \( I_{AxB}(x, y) \)

\( P_{YX} = E_Z[P_{Y|Z} \otimes P_{X|Z}] \)
Characterization of conditional independence

**Theorem**
Define the augmented variable \( \tilde{X} = (X, Z) \) and define a kernel on \( \Omega_X \times \Omega_Z \) by
\[
k_{\tilde{X}} = k_X k_Z
\]
Under (A),
\[
\Sigma_{Y|\tilde{X}|Z} = O \iff X \indep Y \mid Z
\]
\[
\Sigma_{Y|\tilde{X}|Z} = O \iff \Sigma_{\tilde{Y}|X|Z} = O \iff \Sigma_{\tilde{Y}|\tilde{X}|Z} = O \iff X \indep Y \mid Z
\]

**proof**)
\[
\Sigma_{Y|[X,Z]|Z} = O \implies p(x, y, z') = \int p(x, z' \mid z)p(y \mid z)p(z)dz
\]
where \( p(x, z' \mid z) = p(x \mid z)\delta(z'-z) \)
\[
\iff p(x, y, z') = p(x \mid z')p(y \mid z')p(z')
\]
i.e. \( p(x, y \mid z') = p(x \mid z')p(y \mid z') \)
Normalized Cond. Covariance

- **Normalized conditional cross-covariance operator**

  **Definition**

  \[
  W_{YX|Z} = \Sigma^{-1/2}_{YY} \Sigma_{YX|Z} \Sigma^{-1/2}_{XX} = \Sigma^{-1/2}_{YY} \left( \Sigma_{YX} - \Sigma_{YZ} \Sigma_{ZZ}^{-1} \Sigma_{ZX} \right) \Sigma^{-1/2}_{XX}
  \]

  More rigorously,

  \[
  W_{YX|Z} \equiv W_{YX} - W_{YZ} W_{ZX}
  \]

  Recall: \( \Sigma_{YX} = \Sigma_{YY}^{1/2} W_{YX} \Sigma_{XX}^{1/2} \)

- **Conditional independence**

  Under the assumption (A),

  \[
  W_{YX|Z} = O \quad \iff \quad X \perp Y \mid Z
  \]
Conditional Dependence Measure

– HS Normalized Conditional Independence Criteria

$$HSNCIC = \| W_{XY|Z} \|_{HS}^2$$

$$HSNCIC = 0 \iff X \perp Y \mid Z$$

– Hilbert-Schmidt norm of an operator

$$A : H_1 \to H_2$$ operator on a Hilbert space

$$A$$ is called Hilbert-Schmidt if for complete orthonormal systems $$\{ \varphi_i \}$$ of $$H_1$$ and $$\{ \psi_j \}$$ of $$H_2$$

$$\sum_j \sum_i \langle \psi_j, A \varphi_i \rangle^2 < \infty.$$ 

Hilbert-Schmidt norm is defined by

$$\| A \|_{HS}^2 = \sum_j \sum_i \langle \psi_j, A \varphi_i \rangle^2$$
c.f. Frobenius norm of a matrix
Kernel-free Expression

Theorem
Assume

\[ P_{XY} \text{ and } E_Z[P_{YZ} \otimes P_{XZ}] \text{ have density } p_{XY}(x, y) \text{ and } p_{X \perp Y|Z}(x, y), \text{ resp.} \]

\[ H_Z + \mathbb{R} \text{ and } H_X \otimes H_Y + \mathbb{R} \text{ are dense in } L^2(P_Z) \text{ and } L^2(P_X \otimes P_Y), \text{ resp.} \]

\[ W_{YX} \text{ and } W_{YZ} W_{ZX} \text{ are Hilbert-Schmidt.} \]

Then,

\[
\| W_{YX|Z} \|^2_{HS} = \int \int \left( \frac{p_{XY}(x, y) - p_{X \perp Y|Z}(x, y)}{p_X(x)p_Y(y)} \right)^2 p_X(x)p_Y(y) dx dy
\]

In the special case of \( Z = \phi \)

\[
\| W_{YX} \|^2_{HS} = \int \int \left( \frac{p_{XY}(x, y)}{p_X(x)p_Y(y)} - 1 \right)^2 p_X(x)p_Y(y) dx dy
\]

- Kernel-free expression, though the definitions are given by kernels!
– Kernel-free value is reasonable as a “measure” of dependence. c.f. If unnormalized operators are used, the measures do depend on the choice of kernel (HSIC, Gretton et al. ALT2005)

– In the unconditional case,
\[ \text{HS-NIC} = \| W_{yx} \|_{HS}^2 \]
is equal to the mean square contingency, which is one of the popular measures of dependence.

– In the conditional case, if we use the augmented variables
\[
\| W_{yx|z} \|_{HS}^2 = \iint \left( \frac{p_{xyz}(x,y,z) - p_{x|z}(x|z)p_{y|z}(y|z)p_Z(z)}{p_{xz}(x,z)p_{yz}(y,z)} \right)^2 p_{xz}(x,z)p_{yz}(y,z)dx dy dz
\]
(conditional mean square contingency)
– Key idea of the proof

By the eigendecomposition of $\Sigma_{XX}$ and $\Sigma_{YY}$, we have CONS $\{\varphi_i\}$ of $H_X$ and $\{\psi_j\}$ of $H_Y$ such that

$$\Sigma_{XX} \varphi_i = \lambda_i \varphi_i, \quad \Sigma_{YY} \psi_j = \nu_j \psi_j \quad (\lambda_i \geq 0, \nu_j \geq 0)$$

Define

$$\tilde{\varphi}_i = \frac{\varphi_i - E[\varphi_i]}{\sqrt{\lambda_i}}, \quad \tilde{\psi}_j = \frac{\psi_j - E[\psi_j]}{\sqrt{\nu_i}}$$

By the denseness assumption, $\{1\} \cup \{\tilde{\varphi}_i \tilde{\psi}_j\}_{i,j}$ is CONS of $L^2(P_X \otimes P_Y)$

$$\sum_{i,j} \langle \psi_j, W_{XX} \varphi_i \rangle^2 = \sum_{i,j} \langle \Sigma^{-1/2}_{YY} \psi_j, \Sigma_{XX} \Sigma^{-1/2}_{YY} \varphi_i \rangle^2 = \sum_{i,j} \left( \frac{\psi_j}{\sqrt{\nu_j}}, \Sigma_{XX} \frac{\varphi_i}{\sqrt{\lambda_i}} \right)^2$$

$$= \sum_{i,j} E_{XY} \left[ \tilde{\psi}_j (Y) \tilde{\varphi}_i (X) \right]^2 = \sum_{i,j} \left( \tilde{\psi}_j (Y) \tilde{\varphi}_i (X), \frac{p_{XY}}{p_X p_Y} \right)^2$$

$$= \left\| \frac{p_{XY}}{p_X p_Y} \right\|_{L^2(P_X \otimes P_Y)}^2 - 1$$

etc.
Empirical Measures

- Empirical estimation is straightforward with the kernel method.

- Inversion → regularization: \[ \Sigma_{XX}^{-1} \rightarrow (\Sigma_{XX} + \varepsilon I)^{-1} \]

- Replace the covariances in \( W_{XX} = \Sigma_{YY}^{-1/2} \Sigma_{YY} \Sigma_{XX}^{-1/2} \) by the empirical ones given by the data \( \Phi_X(X_1), \ldots, \Phi_X(X_N) \) and \( \Phi_Y(Y_1), \ldots, \Phi_Y(Y_N) \)

\[
H_{SNIC}^\text{emp} = \text{Tr}[R_X R_Y] \quad \text{(dependence measure)}
\]

\[
H_{SNICIC}^\text{emp} = \text{Tr}[R_{\tilde{X}} R_{\tilde{Y}} - 2 R_{\tilde{X}} R_{\tilde{Y}} R_Z + R_{\tilde{X}} R_Z R_{\tilde{Y}} R_Z]
\]

(conditional dependence measure)

where \( R_{\tilde{X}} \equiv G_{\tilde{X}} (G_{\tilde{X}} + N \varepsilon_N I_N)^{-1} \) etc.

- \( H_{SNIC}^\text{emp} \) and \( H_{SNICIC}^\text{emp} \) give kernel estimates for the mean square contingency and conditional mean square contingency, resp.
Relation with Other Measures

- **Mutual Information**

\[
MI(X, Y) = \int \int p_{XY}(x, y) \log \frac{p_{XY}(x, y)}{p_X(x)p_Y(y)} d\mu_X(x)d\mu_Y(y)
\]

- **MI and HSNIC**

\[
HSNIC(X, Y) \leq MI(X, Y)
\]

\[
\therefore HSNIC = \int \int p_{XY}(x, y)\left(\frac{p_{XY}(x, y)}{p_X(x)p_Y(y)} - 1\right)d\mu_1(x)d\mu_2(y)
\leq \int \int p_{XY}(x, y)\log \frac{p_{XY}(x, y)}{p_X(x)p_Y(y)} d\mu_1(x)d\mu_2(y) = MI
\]

\[
(\log z \leq z - 1)
\]
– **Mutual Information:**
  - Information-theoretic meaning.
  - Estimation is not straightforward for continuous variables. Explicit estimation of p.d.f. is difficult for high-dimensional data.
    - Parzen-window is sensitive to the band-width.
    - Partitioning may cause a large number of bins.
  - Some advanced methods: e.g. k-NN approach (Kraskov et al. 2004, Ku&Fine 2005).

– **Kernel method:**
  - Explicit estimation of p.d.f. is not required;
    - the dimension of data does not appear explicitly, but it is influential in practice.
  - Kernel / kernel parameters must be chosen.
Theorem (FGSS2007)

Assume that $W_{YX|Z}$ is Hilbert-Schmidt, and the regularization coefficient satisfies

$\varepsilon_N \to 0 \quad N^{1/3} \varepsilon_N \to \infty.$

Then,

$$\left\| \hat{W}^{(N)}_{YX|Z} - W_{YX|Z} \right\|_{HS} \to 0 \quad (N \to \infty)$$

In particular,

$$\left\| \hat{W}^{(N)}_{YX|Z} \right\|_{HS} \to \left\| W_{YX|Z} \right\|_{HS} \quad (N \to \infty)$$

i.e. $\text{HSNCIC}_{\text{emp}}$ ($\text{HSNIC}_{\text{emp}}$) converges to the population value $\text{HSNCIC}$ ($\text{HSNIC}$, resp).
How to choose a kernel?

- Empirical estimates still depend on the choice of kernels.
- For unsupervised problems, such as independence measures, there are no theoretically reasonable methods.
- Some heuristic methods which work:
  - Heuristics for Gaussian kernels
    \[
    \sigma = \text{median} \left\{ \left\| X_i - X_j \right\| \mid i \neq j \right\}
    \]
  - Speed of asymptotic convergence
    \[
    \lim_{N \to \infty} \text{Var} \left[ N \times HSNIC_{emp}^{(N)} \right] = 2 \left\| \Sigma_{XX} \right\|_{HS}^2 \left\| \Sigma_{YY} \right\|_{HS}^2 \quad \text{under independence}
    \]

Compare the bootstrapped variance and the theoretical one, and choose the parameter to give the minimum discrepancy.
Application to Independence Test

- Toy example

They are all uncorrelated, but dependent for $0 < \theta < \pi/2$
N = 200.
Permutation test is used.

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<th>Angle</th>
<th>0.0</th>
<th>4.5</th>
<th>9.0</th>
<th>13.5</th>
<th>18.0</th>
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<td>HSIC (Median)</td>
<td>93</td>
<td>92</td>
<td>63</td>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>HSIC (Asymp. Var.)</td>
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<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>HSNIC ($\varepsilon = 10^4$, Median)</td>
<td>94</td>
<td>23</td>
<td>0</td>
<td>0</td>
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<td>0</td>
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<td>0</td>
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<tr>
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<tr>
<td>HSNIC (Asymp. Var.)</td>
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<tr>
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</tbody>
</table>

# acceptance of independence out of 100 tests (significance level = 5%)
**Cond. Independence Test**

- **Permutation test with the kernel measure**

\[ T_N = \left\| \Sigma_{YX|Z}^{(N)} \right\|_{HS}^2 \quad \text{or} \quad T_N = \left\| \hat{W}_{YX|Z}^{(N)} \right\|_{HS}^2 \]

- If \( Z \) takes values in a finite set \( \{1, \ldots, L\} \), set \( A_\ell = \{i \mid Z_i = \ell\} \) \( (\ell = 1, \ldots, L) \), otherwise, partition the values of \( Z \) into \( L \) subsets \( C_1, \ldots, C_L \), and set \( A_\ell = \{i \mid Z_i \in C_\ell\} \) \( (\ell = 1, \ldots, L) \).

- Repeat the following process \( B \) times: \( (b = 1, \ldots, B) \)
  1. Generate pseudo cond. independent data \( D^{(b)} \) by permuting \( X \) data within each \( A_\ell \).
  2. Compute \( T_N^{(b)} \) for the data \( D^{(b)} \).

  → Approximate null distribution under cond. indep. assumption

- Set the threshold by the \( (1-\alpha) \)-percentile of the empirical distributions of \( T_N^{(b)} \).
Kernel Method for Causality of Time Series

Causality by conditional independence

- Nonlinear extension of Granger causality

  \( X \) is NOT a cause of \( Y \) if

  \[
  p(Y_t \mid Y_{t-1}, \ldots, Y_{t-p}, X_{t-1}, \ldots, X_{t-p}) = p(Y_t \mid Y_{t-1}, \ldots, Y_{t-p})
  \]

  \( \iff \)

  \[
  Y_t \perp X_{t-1}, \ldots, X_{t-p} \mid Y_{t-1}, \ldots, Y_{t-p}
  \]

- Kernel measures for causality

  \[
  HSNCIC = \left\|
  \hat{\mathcal{W}}_{\hat{Y}_{X_p} \mid Y_p}^{(N-p+1)}
  \right\|_{HS}^2
  \]

  \[
  X_p = \{(X_{t-1}, X_{t-2}, \ldots, X_{t-p}) \in \mathbb{R}^p \mid t = p + 1, \ldots, N\}
  \]

  \[
  Y_p = \{(Y_{t-1}, Y_{t-2}, \ldots, Y_{t-p}) \in \mathbb{R}^p \mid t = p + 1, \ldots, N\}
  \]
Example: Causality of Time-Series

- **Coupled Hénon map**
  
  \( X, Y: \)

  \[
  \begin{align*}
  x_1(t+1) &= 1.4 - x_1(t)^2 + 0.3x_2(t) \\
  x_2(t+1) &= x_1(t)
  \end{align*}
  \]

  \[
  \begin{align*}
  y_1(t+1) &= 1.4 - \left\{ \gamma x_1(t)y_1(t) + (1-\gamma)y_1(t)^2 \right\} + 0.1y_2(t) \\
  y_2(t+1) &= y_1(t)
  \end{align*}
  \]

  \( x_1 - y_1 \)  
  \( \gamma = 0 \)  
  \( \gamma = 0.25 \)  
  \( \gamma = 0.8 \)
Causality of coupled Hénon map

- $X$ is a cause of $Y$ if $\gamma > 0$. \[ Y_t \not\rightarrow X_{t-1}, \ldots, X_{t-p} \mid Y_{t-1}, \ldots, Y_{t-p} \]
- $Y$ is not a cause of $X$ for all $\gamma$. \[ X_t \not\leftarrow Y_{t-1}, \ldots, Y_{t-p} \mid X_{t-1}, \ldots, X_{t-p} \]
- Permutation tests for non-causality with \[ HSNCIC = \left\| \hat{W}_{YX}^{(N-p+1)} \right\|_{HS}^2 \]

<table>
<thead>
<tr>
<th>N = 100</th>
<th>$x_1 - y_1$</th>
<th>$H_0$: $Y_t$ is not a cause of $X_{t+1}$</th>
<th>$H_0$: $X_t$ is not a cause of $Y_{t+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$</td>
<td>0.0 0.1 0.2 0.3 0.4 0.5 0.6</td>
<td>0.0 0.1 0.2 0.3 0.4 0.5 0.6</td>
<td></td>
</tr>
<tr>
<td>HSNCIC</td>
<td>94 88 81 63 86 77 62</td>
<td>97 0 0 0 0 0 0</td>
<td></td>
</tr>
<tr>
<td>Granger</td>
<td>92 96 95 90 90 94 93</td>
<td>96 92 85 45 13 2 3</td>
<td></td>
</tr>
</tbody>
</table>

1-dimensional independent noise is added to $X(t)$ and $Y(t)$.

| HSNCIC   | 97 96 93 85 81 68 75 | 96 0 0 0 0 0 0 |

Number of times accepting $H_0$ among 100 datasets ($\alpha = 5\%$)
Concluding Remarks

Kernel dependence measures
- The normalized (conditional) covariance on RKHS gives kernel-free measures of dependence in population.
- The Gram matrix expression gives the p.d.-kernel estimate of the (conditional) mean square contingency.
- Comparably reliable methods for conditional independence test.

Future directions
- More empirical studies
- More theory on kernel choice
- Application to causal inference (Sun et al., 2007).